```
data_lach5

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;
The (CH2)3Br group at the top of the structure is disordered by
symmetry over three sites. This results in
the atoms having large U values especially the Br.
Some of the atoms at the ends of the NBu4 cation are large due to
disorder.
;

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;
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;
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3Br)]
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 'C63 H141 Br N3 O37 P Si4 W9'
_chemical_formula_weight          3410.68

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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0492   0.0322
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Si'  'Si'   0.2541   0.3302
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 'P'  'P'   0.2955   0.4335
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 'W'  'W'  -5.4734   5.5774
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 'N'  'N'   0.0311   0.0180
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Br'  'Br'  -0.6763   1.2805
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 '-y, x-y, z'
 '-x+y, -x, z'
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 'x, x-y, z+1/2'
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 'x+2/3, y+1/3, z+1/3'
 '-y+2/3, x-y+1/3, z+1/3'
 '-x+y+2/3, -x+1/3, z+1/3'
 '-x+y+2/3, y+1/3, z+5/6'
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 'x+1/3, y+2/3, z+2/3'
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 '-y+1/3, x-y+2/3, z+2/3'
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 'x+1/3, x-y+2/3, z+7/6'
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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor
wR and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
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 'calc w=1/[\s^2^(Fo^2^)+(0.0359P)^2^+0.0000P] where P=(Fo^2^+2Fc^2
^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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 'Flack H D (1983), Acta Cryst. A39, 876-881'
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C2 C 0.0921(12) 0.2390(16) 0.6727(8) 0.274(14) Uani 1 1 d DU . .
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H2A H 0.0518 0.2339 0.6847 0.410 Uiso 1 1 calc R . .
H2B H 0.0789 0.2024 0.6553 0.410 Uiso 1 1 calc R . .
H2C H 0.1152 0.2825 0.6603 0.410 Uiso 1 1 calc R . .
C3 C 0.1683(13) 0.3007(9) 0.7237(6) 0.217(11) Uani 1 1 d DU . .
H3A H 0.1998 0.3007 0.7415 0.326 Uiso 1 1 calc R . .
H3B H 0.1311 0.3020 0.7360 0.326 Uiso 1 1 calc R . .
H3C H 0.1921 0.3405 0.7083 0.326 Uiso 1 1 calc R . .
C4 C 0.2068(14) 0.2419(14) 0.6836(7) 0.222(12) Uani 1 1 d U . .
H4A H 0.2352 0.2401 0.7027 0.333 Uiso 1 1 calc R . .
H4B H 0.2318 0.2849 0.6707 0.333 Uiso 1 1 calc R . .
H4C H 0.1946 0.2045 0.6668 0.333 Uiso 1 1 calc R . .
C8 C 0.2211(8) 0.3643(7) 0.9046(5) 0.104(4) Uani 1 1 d U . .
H8A H 0.2695 0.3938 0.9104 0.124 Uiso 1 1 calc R . .
H8B H 0.1965 0.3862 0.9144 0.124 Uiso 1 1 calc R . .
C9 C 0.2126(12) 0.3595(11) 0.8630(6) 0.152(7) Uani 1 1 d DU . .
H9A H 0.2393 0.3405 0.8523 0.182 Uiso 1 1 calc R . .
H9B H 0.1646 0.3300 0.8565 0.182 Uiso 1 1 calc R . .
C10 C 0.2390(14) 0.4334(13) 0.8490(7) 0.196(11) Uani 1 1 d DU . .
H10A H 0.2866 0.4634 0.8561 0.235 Uiso 1 1 calc R . .
H10B H 0.2113 0.4519 0.8589 0.235 Uiso 1 1 calc R . .
C11 C 0.2321(17) 0.4273(15) 0.8068(7) 0.214(12) Uani 1 1 d DU . .
H11A H 0.2473 0.4720 0.7964 0.320 Uiso 1 1 calc R . .
H11B H 0.1848 0.3969 0.8003 0.320 Uiso 1 1 calc R . .
H11C H 0.2599 0.4092 0.7975 0.320 Uiso 1 1 calc R . .
C12 C 0.2362(9) 0.2621(7) 0.9091(5) 0.109(4) Uani 1 1 d U . .
H12A H 0.2195 0.2180 0.9212 0.131 Uiso 1 1 calc R . .
H12B H 0.2260 0.2530 0.8833 0.131 Uiso 1 1 calc R . .
C13 C 0.3124(10) 0.3026(9) 0.9135(5) 0.126(5) Uani 1 1 d U . .
H13A H 0.3301 0.3455 0.9002 0.152 Uiso 1 1 calc R . .
H13B H 0.3233 0.3139 0.9392 0.152 Uiso 1 1 calc R . .
C14 C 0.3473(12) 0.2660(12) 0.9006(6) 0.158(8) Uani 1 1 d U . .
H14A H 0.3340 0.2522 0.8754 0.190 Uiso 1 1 calc R . .
H14B H 0.3314 0.2243 0.9150 0.190 Uiso 1 1 calc R . .
C15 C 0.4259(13) 0.3081(14) 0.9028(8) 0.219(15) Uani 1 1 d U . .
H15A H 0.4450 0.2805 0.8945 0.328 Uiso 1 1 calc R . .
H15B H 0.4396 0.3220 0.9276 0.328 Uiso 1 1 calc R . .
H15C H 0.4424 0.3482 0.8876 0.328 Uiso 1 1 calc R . .
C17 C 0.1925(11) 0.2526(10) 0.9885(5) 0.137(6) Uani 1 1 d U . .
H17A H 0.2188 0.2311 0.9808 0.165 Uiso 1 1 calc R . .
H17B H 0.1440 0.2184 0.9866 0.165 Uiso 1 1 calc R . .
C18 C 0.2101(13) 0.2757(13) 1.0297(6) 0.198(11) Uani 1 1 d DU . .
H18A H 0.2592 0.3075 1.0318 0.238 Uiso 1 1 calc R . .
H18B H 0.1864 0.3002 1.0368 0.238 Uiso 1 1 calc R . .
C19 C 0.1900(14) 0.2156(14) 1.0564(8) 0.246(14) Uani 1 1 d DU . .
H19A H 0.2027 0.2333 1.0808 0.369 Uiso 1 1 calc R . .
H19B H 0.2136 0.1914 1.0499 0.369 Uiso 1 1 calc R . .
H19C H 0.1412 0.1847 1.0553 0.369 Uiso 1 1 calc R . .
C20 C 0.1223(8) 0.2473(8) 0.9153(5) 0.133(6) Uani 1 1 d DU . .
H20A H 0.1085 0.2043 0.9280 0.159 Uiso 1 1 calc R . .
H20B H 0.1190 0.2377 0.8893 0.159 Uiso 1 1 calc R . .
C21 C 0.0692(8) 0.2706(10) 0.9248(7) 0.174(10) Uani 1 1 d DU . .
H21A H 0.0929 0.3206 0.9240 0.209 Uiso 1 1 calc R . .
H21B H 0.0343 0.2537 0.9058 0.209 Uiso 1 1 calc R . .
C22 C 0.0382(12) 0.2509(14) 0.9562(9) 0.216(13) Uani 1 1 d DU . .
H22A H 0.0696 0.2765 0.9759 0.259 Uiso 1 1 calc R . .
H22B H 0.0215 0.2022 0.9599 0.259 Uiso 1 1 calc R . .
C23 C -0.0252(12) 0.2656(15) 0.9551(9) 0.258(17) Uani 1 1 d DU . .
H23A H -0.0496 0.2519 0.9779 0.387 Uiso 1 1 calc R . .
H23B H -0.0558 0.2398 0.9355 0.387 Uiso 1 1 calc R . .
H23C H -0.0078 0.3139 0.9512 0.387 Uiso 1 1 calc R . .
C16 C 0.2081(9) 0.3110(7) 0.9636(4) 0.110(4) Uani 1 1 d U . .
H16A H 0.2562 0.3456 0.9666 0.131 Uiso 1 1 calc R . .
H16B H 0.1810 0.3315 0.9714 0.131 Uiso 1 1 calc R . .
O1 O 0.2496(4) 0.2071(4) 0.8144(2) 0.0659(19) Uani 1 1 d U . .
O2 O 0.1706(3) 0.0679(3) 0.79961(19) 0.0519(16) Uani 1 1 d U . .
O3 O 0.0448(3) 0.0733(3) 0.80013(17) 0.0440(13) Uani 1 1 d U . .

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O4 O 0.1223(3) 0.2027(3) 0.8182(2) 0.0527(15) Uani 1 1 d U . .
O5 O 0.0236(4) 0.2424(4) 0.8160(2) 0.071(2) Uani 1 1 d U . .
O6 O 0.0000 0.0000 0.8553(3) 0.037(2) Uani 1 3 d SU . .
O7 O 0.1417(3) 0.1160(3) 0.85792(19) 0.0492(14) Uani 1 1 d U . .
O8 O 0.0068(3) 0.1321(3) 0.85841(18) 0.0490(14) Uani 1 1 d U . .
O9 O -0.0699(4) 0.0931(4) 0.9251(2) 0.070(2) Uani 1 1 d U . .
O10 O 0.0465(3) 0.0796(3) 0.91190(19) 0.0543(16) Uani 1 1 d U . .
O11 O 0.1554(4) 0.1602(3) 0.75797(19) 0.0581(15) Uani 1 1 d U . .
O12 O 0.0452(4) 0.1752(4) 0.7590(2) 0.0644(17) Uani 1 1 d U . .
O13 O 0.0529(5) 0.0884(5) 0.7103(3) 0.101(3) Uani 1 1 d U . .
Si1 Si 0.09623(18) 0.16210(18) 0.73231(9) 0.0696(8) Uani 1 1 d U . .
P1 P 0.0000 0.0000 0.81241(11) 0.0326(7) Uani 1 3 d SU . .
W1 W 0.16482(2) 0.14714(2) 0.808478(11) 0.04981(13) Uani 1 1 d U . .
W2 W 0.02716(2) 0.16882(2) 0.810079(11) 0.04981(13) Uani 1 1 d U . .
W3 W -0.04269(2) 0.05778(2) 0.892415(15) 0.04688(12) Uani 1 1 d U . .
N1 N 0.1951(6) 0.2949(5) 0.9240(4) 0.104(3) Uani 1 1 d U . .
Si2 Si 0.0000 0.0000 0.6888(12) 0.266 Uiso 0.48(2) 3 d SPDU . .
C5 C 0.0000 0.0000 0.6314(12) 0.120(10) Uani 0.48(2) 3 d SPDU . .
H5A H 0.0475 0.0347 0.6266 0.144 Uiso 0.162(7) 1 calc PR . .
H5B H -0.0017 -0.0434 0.6266 0.144 Uiso 0.162(7) 1 calc PR . .
Br1 Br -0.046(4) 0.006(6) 0.5243(13) 0.540 Uiso 0.162(7) 1 d PDU . .
C7 C 0.0000 0.0000 0.5625(13) 0.138(13) Uani 0.48(2) 3 d SPDU . .
H7A H -0.0016 -0.0441 0.5624 0.166 Uiso 0.162(7) 1 calc PR . .
H7B H 0.0478 0.0365 0.5618 0.166 Uiso 0.162(7) 1 calc PR . .
C6 C -0.035(5) 0.007(7) 0.5962(12) 0.132(14) Uani 0.162(7) 1 d PDU .
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H6A H -0.0836 -0.0289 0.5960 0.159 Uiso 0.162(7) 1 calc PR . .
H6B H -0.0331 0.0511 0.5960 0.159 Uiso 0.162(7) 1 calc PR . .

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C2 0.21(2) 0.29(3) 0.28(3) 0.211(19) -0.011(17) 0.09(2)
C3 0.33(3) 0.086(8) 0.200(19) 0.065(9) 0.116(15) 0.075(14)
C4 0.24(2) 0.26(3) 0.23(2) 0.152(19) 0.174(18) 0.18(2)
C8 0.097(10) 0.076(7) 0.136(8) -0.041(6) -0.017(9) 0.042(7)
C9 0.163(19) 0.157(14) 0.125(9) -0.050(9) -0.029(14) 0.073(16)
C10 0.18(2) 0.204(18) 0.162(14) 0.020(15) -0.032(18) 0.07(2)
C11 0.26(3) 0.24(3) 0.154(14) 0.004(16) 0.03(2) 0.14(3)
C12 0.138(8) 0.064(8) 0.121(12) -0.029(8) 0.003(10) 0.047(8)
C13 0.136(9) 0.119(13) 0.137(15) -0.013(11) 0.003(12) 0.074(10)
C14 0.183(14) 0.17(2) 0.17(2) -0.038(16) -0.028(17) 0.129(16)
C15 0.185(15) 0.25(3) 0.27(3) -0.11(3) -0.01(2) 0.14(2)
C17 0.142(16) 0.129(14) 0.172(11) -0.015(10) -0.019(14) 0.090(14)
C18 0.16(2) 0.24(3) 0.143(11) 0.032(13) 0.033(15) 0.06(2)
C19 0.25(3) 0.32(4) 0.225(19) 0.08(2) 0.00(3) 0.19(3)
C20 0.103(8) 0.096(10) 0.139(14) -0.071(10) -0.002(8) 0.005(7)
C21 0.083(9) 0.152(18) 0.22(2) -0.093(16) 0.009(12) 0.005(10)
C22 0.16(2) 0.20(3) 0.27(3) -0.04(2) 0.07(2) 0.074(19)
C23 0.14(2) 0.29(3) 0.32(4) -0.12(3) 0.03(2) 0.09(2)
C16 0.104(11) 0.076(8) 0.127(8) -0.046(6) -0.007(8) 0.028(9)
O1 0.043(3) 0.059(4) 0.088(5) 0.009(4) 0.005(3) 0.020(3)
O2 0.041(3) 0.051(3) 0.061(4) 0.010(3) 0.012(3) 0.021(3)
O3 0.039(3) 0.034(3) 0.055(4) 0.003(2) -0.003(3) 0.015(2)
O4 0.054(3) 0.031(3) 0.069(4) 0.003(3) -0.002(3) 0.018(3)
O5 0.074(5) 0.053(4) 0.092(6) 0.008(4) 0.006(4) 0.036(4)
O6 0.031(3) 0.031(3) 0.049(5) 0.000 0.000 0.0153(14)
O7 0.040(3) 0.040(3) 0.065(4) -0.007(3) -0.008(3) 0.017(3)
O8 0.055(4) 0.038(3) 0.058(4) -0.013(2) -0.009(3) 0.026(3)
O9 0.068(5) 0.076(5) 0.067(5) -0.016(4) 0.002(4) 0.038(4)
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O10 0.052(4) 0.055(4) 0.056(4) -0.006(3) -0.009(3) 0.026(3)
O11 0.056(4) 0.047(4) 0.068(4) 0.009(3) 0.011(3) 0.024(3)
O12 0.063(4) 0.058(4) 0.073(4) 0.016(3) 0.000(3) 0.031(4)
O13 0.098(7) 0.099(6) 0.108(8) -0.028(5) -0.021(5) 0.050(5)
Si1 0.080(2) 0.072(2) 0.0605(19) 0.0124(15) 0.0043(15) 0.0409(17)
P1 0.0299(10) 0.0299(10) 0.038(2) 0.000 0.000 0.0149(5)
W1 0.0374(2) 0.0407(2) 0.0642(4) 0.0066(2) 0.0029(2) 0.01419(19)
W2 0.0504(3) 0.0387(3) 0.0632(3) 0.0029(2) -0.0031(2) 0.0244(2)
W3 0.0472(3) 0.0471(3) 0.0489(2) -0.0056(2) 0.0009(2) 0.0255(2)
N1 0.092(6) 0.055(5) 0.132(7) -0.050(5) -0.001(7) 0.011(5)
C5 0.125(14) 0.125(14) 0.110(11) 0.000 0.000 0.062(7)
C7 0.147(16) 0.147(16) 0.121(13) 0.000 0.000 0.074(8)
C6 0.13(2) 0.14(3) 0.116(17) -0.001(17) -0.006(12) 0.060(19)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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C1 Si1 1.850(14) . ?
C8 N1 1.53(2) . ?
C8 C9 1.53(2) . ?
C9 C10 1.542(17) . ?
C10 C11 1.553(17) . ?
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C14 C15 1.53(3) . ?
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C17 C18 1.58(3) . ?
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C21 C22 1.30(3) . ?
C22 C23 1.612(18) . ?
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O3 P1 1.503(6) . ?
O3 W1 2.369(6) . ?
O3 W2 2.391(6) . ?
O4 W2 1.895(6) . ?
O4 W1 1.942(6) . ?
O5 W2 1.703(7) . ?
O6 P1 1.569(11) . ?
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O6 W3 2.381(6) 3 ?
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O7 W1 1.914(7) . ?
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O8 W3 1.925(7) . ?
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O10 W3 1.911(7) 3 ?
O10 W3 1.940(6) . ?
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O11 W1 1.898(7) . ?
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O12 W2 1.903(8) . ?
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P1 O3 1.503(6) 2 ?
P1 O3 1.503(6) 3 ?
W2 O2 1.930(6) 2 ?
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Si2 O13 1.90(2) 3 ?
Si2 O13 1.90(2) 2 ?
C5 C6 1.56(2) . ?
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C4 C1 Si1 112.5(11) . . ?
C3 C1 Si1 106.6(11) . . ?
N1 C8 C9 114.5(12) . . ?
C10 C9 C8 106.5(16) . . ?
C9 C10 C11 105(2) . . ?
C13 C12 N1 116.7(11) . . ?
C14 C13 C12 113.2(17) . . ?
C13 C14 C15 114(2) . . ?
C16 C17 C18 112.7(16) . . ?
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N1 C20 C21 117.7(12) . . ?
C22 C21 C20 117(2) . . ?
C21 C22 C23 106(3) . . ?
C17 C16 N1 116.9(13) . . ?
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P1 O3 W2 127.8(3) . . ?
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W2 O4 W1 121.9(3) . . ?
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W3 O6 W3 90.7(3) 3 . ?
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W2 O8 W3 152.0(3) . . ?
W3 O10 W3 123.3(4) 3 . ?
Si1 O11 W1 135.5(4) . . ?
Si1 O12 W2 135.5(4) . . ?
Si1 O13 Si2 175.2(15) . . ?
O12 Si1 O11 108.0(4) . . ?
O12 Si1 O13 110.9(5) . . ?
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O11 Si1 C1 108.0(6) . . ?
O13 Si1 C1 111.8(7) . . ?
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O1 W1 O3 174.2(3) . . ?
O2 W1 O3 84.7(2) . . ?
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O4 W1 O3 73.9(2) . . ?
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O5 W2 O12 99.5(3) . . ?
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O5 W2 O8 100.4(3) . . ?
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O12 W2 O8 159.9(3) . . ?
O5 W2 O2 101.6(3) . 2 ?
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O12 W2 O2 88.5(3) . 2 ?
O8 W2 O2 85.3(3) . 2 ?
O5 W2 O3 173.9(3) . . ?
O4 W2 O3 74.1(2) . . ?
O12 W2 O3 78.0(3) . . ?
O8 W2 O3 82.3(2) . . ?
O2 W2 O3 84.0(2) 2 . ?
O9 W3 O7 101.4(3) . 2 ?
O9 W3 O10 99.7(3) . 2 ?
O7 W3 O10 90.8(3) 2 2 ?
O9 W3 O8 103.6(3) . . ?
O7 W3 O8 85.0(3) 2 . ?
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O9 W3 O10 100.9(3) . . ?
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O8 W3 O10 86.8(3) . . ?
O9 W3 O6 170.3(3) . . ?
O7 W3 O6 85.6(2) 2 . ?
O10 W3 O6 73.2(2) 2 . ?
O8 W3 O6 83.6(2) . . ?
O10 W3 O6 72.7(3) . . ?
C20 N1 C16 113.4(13) . . ?
C20 N1 C8 111.0(14) . . ?
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C20 N1 C12 106.8(10) . . ?
C16 N1 C12 111.7(14) . . ?
C8 N1 C12 108.0(12) . . ?
C5 Si2 O13 114.4(13) . . ?
C5 Si2 O13 114.4(13) . 3 ?
O13 Si2 O13 104.1(15) . 3 ?
C5 Si2 O13 114.4(13) . 2 ?
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C6 C5 Si2 145.7(14) . . ?
C7 Br1 Br1 57.4(14) . 3 ?
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